Shock-Induced Chemical Reactions in High Explosive Materials

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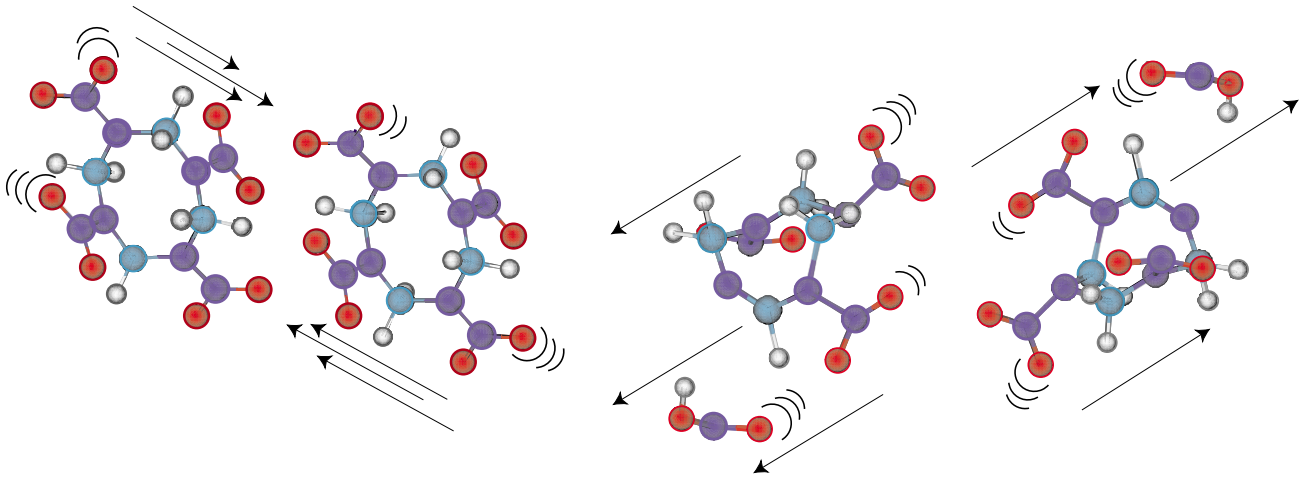
Conventional high explosives (HE) are molecular crystals that release mechanical and thermal energy through chemical reactions when the material is subjected to sufficient mechanical impact. Shock compression of the HE material causes the molecules to collide with each other at high velocities.

We make use of quantum molecular dynamics (QMD) to study the breaking and formation of chemical bonds during a shock-induced collision of HE molecules. In the QMD computational technique all interactions between atoms are evalutated quantum mechanically while their motion is treated by classical mechanics.

The Figure shows the shock-induced collision of two HMX molecules and the resulting chemical reaction which is consistent with experimental observations demonstrating the viability of this approach.

Our results will provide molecular-scale information for improved models describing HE initiation.



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